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Solvation state of iron(III) in aqueous solutions of dimethyl sulfoxide. Complex formation ability of iron(III) with respect to derivatives of sym-triazine and bis(hydrazinocarbonylmethyl) sulfoxide

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Abstract

© 2016, Pleiades Publishing, Ltd.Parameters of the solvation equilibria [Fe(H2O)6]3++nDMSO⇄[Fe(H2O)6−n(DMSO)n]3++nH2O have been determined in aqueous-dimethyl sulfoxide solutions (0–90 vol% DMSO) by means of spectrophotometry and mathematical modeling of equilibria. Iron(III) is not involved in the complex formation with derivatives of sym-triazine: 2,4-diamino-6-(carbamoylmethylsulfinylmethyl)-1,3,5-triazine and 2,4-diamino-6-(acetohydrazidomethylsulfinylmethyl)-1,3,5-triazine in aqueous DMSO medium (40 vol % DMSO). Bis(hydrazinocarbonylmethyl) sulfoxide forms two complexes with iron(III), with 1: 1 and 1: 2 compositions; in contrast to the Cu(II) and Ni(II) complexes, in the iron complexes the ligand exists in the amide form. The most probable structures of the complexes have been revealed by molecular mechanics simulation and (in selected cases) using the DFT/B3LYP/6-31++G(d,p) density functional theory method.

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Keywords

bis(hydrazinocarbonylmethyl) sulfoxide, complex formation, dimethyl sulfoxide, ligand denticity, solvation state, sym-triazine derivative